

Supplementary Material to

Title: Improved Statistical Significance of Clustering

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A Proof of all Theorems

Before giving the proofs of our theorems, we provide the following two lemmas which will be used for our proofs of the theorems.

Lemma 1. *von Neumann's lower bound trace inequality: for d -dimensional positive semi-definite matrices A and B , denote $\lambda_j(A)$ ($j = 1, \dots, d$) as the j th eigenvalue of A , then $\text{trace}(AB) \geq \sum_{j=1}^d \lambda_j(A)\lambda_{d-j+1}(B)$.*

Proof. From von Neumann's trace inequality (Mirsky, 1975), we have

$$\begin{aligned} \text{trace}(A[\lambda_1(B)I - B]) &\leq \sum_j \lambda_j(A)\lambda_j(\lambda_1(B)I - B) \\ &= \sum_j \lambda_j(A)[\lambda_1(B) - \lambda_{d-j+1}(B)] \\ &= \lambda_1(B) \sum_j \lambda_j(A) - \sum_j \lambda_j(A)\lambda_{d-j+1}(B), \end{aligned}$$

which implies the lower bound

$$\text{trace}(AB) \geq \sum_j \lambda_j(A)\lambda_{d-j+1}(B)$$

since

$$\text{trace}(A(\lambda_1(B)I - B)) = \lambda_1(B)\text{trace}(A) - \text{trace}(AB).$$

This completes the proof of Lemma 1.

Define $\alpha = 1/\sigma_N^2$. Now consider the optimization problem

$$\min_{d_1, \dots, d_d} \left[-\sum_{k=1}^d \ln(\alpha - d_k) + \sum_{k=1}^d \tilde{\lambda}_k(\alpha - d_k) \right] \quad (\text{A.1})$$

$$\text{subject to } 0 \leq d_k \leq \alpha, \#\{k : d_k > 0\} \leq l, k = 1, \dots, d. \quad (\text{A.2})$$

Let $\hat{d}_1, \dots, \hat{d}_d$ be the solution to (A.1) (A.2) and $\hat{D} = \text{diag}(\hat{d}_1, \dots, \hat{d}_d)$. Then the following lemma establishes the relationship between \hat{D} and the solution to (7) (8) (9).

Lemma 2. *The solution to (7) (8) (9) is $\tilde{U}(\alpha I - \hat{D})\tilde{U}^T$.*

Proof. Assume that the solution of (A.1) (A.2) leads to an objective value o_1 , and the solution of (7) (8) (9) leads to an objective value o_2 . From von Neumann's lower bound trace inequality, we have

$$\text{trace}(C\tilde{\Sigma}) \geq \sum_{k=1}^d \lambda_k(\tilde{\Sigma})\lambda_{d-k+1}(C) = \sum_{k=1}^d \tilde{\lambda}_k(\alpha - d_k)$$

for the second term of (7), since $\lambda_{d-k+1}(C) = \lambda_{d-k+1}(\alpha - W_0) = \alpha - d_k$. Consequently, we have $o_1 \leq o_2$. The proof is now completed because $\tilde{U}(\alpha I - \hat{D})\tilde{U}^T$ is in the feasible region of (8) and (9) and it can be verified that when plugging it into (7), the objective function reaches o_1 , which must be a minimum of (7) since $o_1 \leq o_2$. This completes the proof of Lemma 2.

With the two lemmas in place, we are now ready to prove Theorem 1.

Proof of Theorem 1: First, note that the optimization problem in (A.1) and (A.2) can be reduced to d subproblems indexed by k :

$$\begin{aligned} \min_{d_k} \left[-\ln(\alpha - d_k) + \tilde{\lambda}_k(\alpha - d_k) \right] & \quad (\text{A.3}) \\ \text{subject to } 0 \leq d_k \leq \alpha. & \end{aligned}$$

Note that when $\tilde{\lambda}_k \leq 1/\alpha = \sigma_N^2$, the objective function (A.3) is increasing in the feasible region. Therefore, we must have $\hat{d}_k = 0$. Otherwise, first order condition leads to $\hat{d}_k = \alpha - 1/\tilde{\lambda}_k$. To sum up, we have

$$\hat{d}_k = (\alpha - 1/\tilde{\lambda}_k)_+.$$

Note that the corresponding minimum

$$-\ln(\alpha - \hat{d}_k) + \tilde{\lambda}_k(\alpha - \hat{d}_k) = -\ln\left(\alpha \wedge \frac{1}{\tilde{\lambda}_k}\right) + (1 \wedge \alpha \tilde{\lambda}_k)$$

is an increasing function of $\tilde{\lambda}_k$, which suggests that the solution to (A.1) (A.2) is

$$\hat{d}_k = \begin{cases} \alpha - 1/\tilde{\lambda}_k & \text{if } k \leq l \text{ and } \tilde{\lambda}_k > \sigma_N^2 \\ 0 & \text{otherwise.} \end{cases}$$

This completes the proof of Theorem 1.

For Theorem 2, we consider an alternative optimization problem to (7), (8), and (11):

$$\min_{d_1, \dots, d_d} \left[-\sum_{k=1}^d \ln(\alpha - d_k) + \sum_{k=1}^d \tilde{\lambda}_k(\alpha - d_k) \right] \quad (\text{A.4})$$

$$\text{subject to } 0 \leq d_k \leq \alpha, \quad \sum d_k \leq M, \quad k = 1, \dots, d. \quad (\text{A.5})$$

Let $\hat{d}_1, \dots, \hat{d}_d$ be the solution to (A.4), (A.5), and $\hat{\Lambda} = \text{diag}(\hat{d}_1, \dots, \hat{d}_d)$. Then we have the following lemma which can be proved in the same fashion as Lemma 2.

Lemma 3. *The solution to (7) (8) (11) is $\tilde{U}(\alpha I - \hat{\Lambda})\tilde{U}^T$.*

Proof of Theorem 2:

To solve (A.4) (A.5), we first write them in a Lagrange form

$$\begin{aligned} \min_{d_1, \dots, d_k} \sum_{k=1}^d [-\ln(\alpha - d_k) + \tilde{\lambda}_k(\alpha - d_k) + \tau d_k] \\ \text{subject to } 0 \leq d_k \leq \alpha, \quad k = 1, \dots, d. \end{aligned}$$

which essentially can be solved as d separate problems. When $\tilde{\lambda}_k \leq \tau + \sigma_N^2$,

$$-\ln(\alpha - d_k) + \tilde{\lambda}_k(\alpha - d_k) + \tau d_k$$

is an increasing function of d_k in the feasible set $[0, \alpha]$. Therefore, $\hat{d}_k = 0$. Otherwise, the first order condition yields

$$\hat{d}_k = \alpha - \frac{1}{\tilde{\lambda}_k - \tau}.$$

In other words,

$$\hat{d}_k = \left(\alpha - \frac{1}{\tilde{\lambda}_k - \tau} \right)_+.$$

It is now clear that the tuning parameters τ and M are related through

$$\sum_{k=1}^d \hat{d}_k = \left(\alpha - \frac{1}{\tilde{\lambda}_k - \tau} \right)_+ = M.$$

From Lemma 3, we have

$$\hat{\lambda}_k = \frac{1}{\alpha - \hat{d}_k} = (\tilde{\lambda}_k - \tau - \sigma_N^2)_+ + \sigma_N^2.$$

This completes the proof of Theorem 2.

Proof of Theorem 3:

Due to rotation invariance, it is enough to consider the situations with diagonal covariance matrix. Let's first calculate the total sum square TSS.

$$\begin{aligned} \text{TSS} &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \|\mathbf{x}\|^2 \phi(\mathbf{x}) dx_1 \cdots dx_d \\ &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \sum_{j=1}^d x_j^2 \left(\prod_{j=1}^d \varphi_{\lambda_j}(x_j) \right) dx_1 \cdots dx_d \\ &= \sum_{j=1}^d \int_{-\infty}^{\infty} x_j^2 \varphi_{\lambda_j}(x_j) dx_j = \sum_{j=1}^d \lambda_j, \end{aligned}$$

where $\phi(\mathbf{x}) = \prod_{j=1}^d \varphi_{\lambda_j}(x_j) = \prod_{j=1}^d \frac{1}{\sqrt{2\pi\lambda_j}} e^{-x_j^2/2\lambda_j}$. Now assume that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$. Then $(1, 0, \dots, 0)^T$ is the direction of the greatest variation. Thus it makes sense to define the 2-means separating plane as the plane which is through $\boldsymbol{\mu} = (0, \dots, 0)^T$ and orthogonal to $(1, 0, \dots, 0)^T$.

Let WSS_1 denote the sum square within Class 1 and WSS_2 the sum square within Class 2. First find center points: $\boldsymbol{\mu}_1 = (\mu_{11}, \mu_{12}, \dots, \mu_{1d})^T$. By symmetry, we have $\mu_{12} = \mu_{13} = \dots = \mu_{1d} = 0$.

$$\mu_{11} = 2 \int_0^\infty x_1 \varphi_{\lambda_1}(x_1) dx_1 = \sqrt{\frac{2\lambda_1}{\pi}}.$$

Here 2 is the normalization factor. So $\boldsymbol{\mu}_1 = \left(\sqrt{\frac{2\lambda_1}{\pi}}, 0, \dots, 0\right)^T$. Similarly, $\boldsymbol{\mu}_2 = \left(-\sqrt{\frac{2\lambda_1}{\pi}}, 0, \dots, 0\right)^T$.

Next

$$\begin{aligned} \text{WSS}_1 &= \int_0^\infty \dots \int_{-\infty}^\infty \|\mathbf{x} - \boldsymbol{\mu}_1\|^2 \phi(\mathbf{x}) dx_1 \dots dx_d \\ &= \int_0^\infty \left(x_1 - \sqrt{\frac{2\lambda_1}{\pi}}\right)^2 \varphi_{\lambda_1}(x_1) dx_1 + \sum_{j=2}^d \int_0^\infty \int_{-\infty}^\infty \dots \int_{-\infty}^\infty x_j^2 \phi(\mathbf{x}) dx_1 \dots dx_d \\ &= \left(\frac{\pi - 2}{2\pi}\right) \lambda_1 + \sum_{j=2}^d \frac{\lambda_j}{2}. \end{aligned}$$

Similarly $\text{WSS}_2 = \text{WSS}_1$. Thus

$$\text{TCI} = \frac{\text{WSS}_1 + \text{WSS}_2}{\text{TSS}} = 1 - \frac{2}{\pi} \frac{\lambda_1}{\sum_{j=1}^d \lambda_j}.$$

This completes of the proof of Theorem 3.

B More Simulated Examples

We perform more simulations in this section. The simulation setting is the same as in Section 3.1 but with different dimensions. Tables A, B, and C summarize the results for $d = 5000$, $d = 300$, and $d = 200$ respectively. As dimension increases, there was less anti-conservatism for the hard method. The sample and the soft methods can control the type-I error in all situations.

References

Mirsky, L. (1975). A trace inequality of John von Neumann. *Monatsh. Math.* 79, 303–306.

Table A: Summary table of empirical SigClust p -value distribution over 100 replications based on four methods under different settings in Simulation 3.1. The mean and the numbers of p -values which are less than 0.05 (denoted as N5) and 0.1 (denoted as N10) are reported (d=5000, n=100).

v	w	True			Sample			Hard			Soft		
		Mean	N5	N10	Mean	N5	N10	Mean	N5	N10	Mean	N5	N10
1000	1	0.55	8	13	0.65	0	0	0.00	100	100	0.47	0	0
200	5	0.39	5	12	0.98	0	0	0.01	98	100	0.65	0	0
100	10	0.36	7	16	1.00	0	0	0.28	5	13	0.80	0	0
40	25	0.29	14	22	1.00	0	0	1.00	0	0	0.97	0	0
20	50	0.22	11	24	1.00	0	0	1.00	0	0	1.00	0	0
10	100	0.20	19	31	1.00	0	0	1.00	0	0	1.00	0	0
200	1	0.54	6	11	0.97	0	0	0.00	100	100	0.42	0	0
100	1	0.58	2	4	1.00	0	0	0.39	5	15	0.44	0	0
50	1	0.51	8	10	1.00	0	0	1.00	0	0	0.81	0	0
40	1	0.50	6	9	1.00	0	0	1.00	0	0	0.98	0	0
30	1	0.50	5	8	1.00	0	0	1.00	0	0	1.00	0	0
20	1	0.48	4	6	1.00	0	0	1.00	0	0	1.00	0	0
10	1	0.21	20	28	1.00	0	0	1.00	0	0	1.00	0	0
50	10	0.35	11	20	1.00	0	0	0.97	0	0	0.84	0	0
40	10	0.38	5	15	1.00	0	0	1.00	0	0	0.92	0	0
30	10	0.26	23	36	1.00	0	0	1.00	0	0	0.98	0	0
20	10	0.36	7	13	1.00	0	0	1.00	0	0	1.00	0	0
10	10	0.22	18	27	1.00	0	0	1.00	0	0	1.00	0	0
50	5	0.41	5	17	1.00	0	0	0.98	0	0	0.78	0	0
40	5	0.41	6	13	1.00	0	0	1.00	0	0	0.91	0	0
30	5	0.35	10	16	1.00	0	0	1.00	0	0	1.00	0	0
20	5	0.35	7	13	1.00	0	0	1.00	0	0	1.00	0	0
10	5	0.24	13	27	1.00	0	0	1.00	0	0	1.00	0	0
50	2	0.47	6	12	1.00	0	0	0.99	0	0	0.78	0	0
40	2	0.44	7	14	1.00	0	0	1.00	0	0	0.95	0	0
30	2	0.50	7	13	1.00	0	0	1.00	0	0	1.00	0	0
20	2	0.43	4	9	1.00	0	0	1.00	0	0	1.00	0	0
10	2	0.24	12	23	1.00	0	0	1.00	0	0	1.00	0	0
5	1	0.14	26	50	1.00	0	0	1.00	0	0	1.00	0	0
3	1	0.13	24	51	1.00	0	0	1.00	0	0	1.00	0	0
1	1	0.14	24	47	1.00	0	0	1.00	0	0	1.00	0	0

Table B: Summary table of empirical SigClust p -value distribution over 100 replications based on four methods under different settings in Simulation 3.1. The mean and the numbers of p -values which are less than 0.05 (denoted as N5) and 0.1 (denoted as N10) are reported (d=300, n=100).

v	w	True			Sample			Hard			Soft		
		Mean	N5	N10	Mean	N5	N10	Mean	N5	N10	Mean	N5	N10
1000	1	0.46	6	18	0.48	4	7	0.04	77	88	0.45	4	9
200	5	0.37	9	14	0.75	0	0	0.30	1	7	0.69	0	0
100	10	0.35	7	12	0.90	0	0	0.52	0	0	0.84	0	0
40	25	0.26	7	24	0.99	0	0	0.84	0	0	0.96	0	0
20	50	0.26	14	26	1.00	0	0	0.97	0	0	0.99	0	0
10	100	0.22	18	34	1.00	0	0	1.00	0	0	1.00	0	0
200	1	0.48	3	5	0.53	0	0	0.00	100	100	0.43	0	0
100	1	0.50	5	15	0.58	0	0	0.00	100	100	0.40	0	1
50	1	0.53	3	9	0.65	0	0	0.00	100	100	0.34	0	2
40	1	0.54	5	7	0.73	0	0	0.00	100	100	0.37	0	2
30	1	0.49	6	9	0.78	0	0	0.00	100	100	0.33	0	2
20	1	0.51	7	11	0.87	0	0	0.01	97	99	0.28	1	3
10	1	0.47	5	12	0.98	0	0	0.17	19	38	0.35	0	0
50	10	0.35	4	11	0.92	0	0	0.32	0	1	0.81	0	0
40	10	0.34	7	15	0.92	0	0	0.26	2	12	0.78	0	0
30	10	0.33	7	15	0.94	0	0	0.21	6	22	0.76	0	0
20	10	0.33	6	15	0.97	0	0	0.16	4	30	0.70	0	0
10	10	0.36	6	11	1.00	0	0	0.31	2	6	0.66	0	0
50	5	0.38	5	10	0.83	0	0	0.05	60	87	0.63	0	0
40	5	0.33	10	13	0.84	0	0	0.04	80	94	0.60	0	0
30	5	0.37	6	11	0.88	0	0	0.03	85	96	0.56	0	0
20	5	0.39	4	13	0.94	0	0	0.04	71	90	0.53	0	0
10	5	0.39	11	18	0.99	0	0	0.18	12	30	0.49	0	0
50	2	0.46	3	6	0.72	0	0	0.00	100	100	0.44	0	0
40	2	0.42	10	15	0.75	0	0	0.00	100	100	0.45	0	0
30	2	0.45	4	6	0.80	0	0	0.01	98	100	0.39	0	1
20	2	0.53	2	4	0.90	0	0	0.02	92	98	0.37	0	0
10	2	0.42	6	14	0.99	0	0	0.15	23	41	0.38	0	0
5	1	0.44	4	7	1.00	0	0	0.95	0	0	0.91	0	0
3	1	0.23	15	23	1.00	0	0	1.00	0	0	1.00	0	0
1	1	0.17	23	38	1.00	0	0	1.00	0	0	1.00	0	0

Table C: Summary table of empirical SigClust p -value distribution over 100 replications based on four methods under different settings in Simulation 3.1. The mean and the numbers of p -values which are less than 0.05 (denoted as N5) and 0.1 (denoted as N10) are reported (d=200, n=100).

v	w	True			Sample			Hard			Soft		
		Mean	N5	N10	Mean	N5	N10	Mean	N5	N10	Mean	N5	N10
1000	1	0.49	5	10	0.50	4	10	0.14	44	62	0.48	6	11
200	5	0.37	3	14	0.76	0	0	0.47	0	0	0.71	0	0
100	10	0.32	10	18	0.87	0	0	0.65	0	0	0.83	0	0
40	25	0.28	9	20	0.98	0	0	0.90	0	0	0.96	0	0
20	50	0.27	14	25	1.00	0	0	0.98	0	0	0.99	0	0
10	100	0.20	21	34	1.00	0	0	1.00	0	0	1.00	0	0
200	1	0.52	3	6	0.55	0	1	0.01	96	99	0.46	0	3
100	1	0.52	5	7	0.60	0	0	0.01	96	99	0.47	0	0
50	1	0.50	6	9	0.62	0	0	0.00	100	100	0.38	0	2
40	1	0.52	5	7	0.64	0	0	0.00	99	100	0.35	0	0
30	1	0.49	4	10	0.69	0	0	0.01	100	100	0.33	0	1
20	1	0.52	9	10	0.77	0	0	0.01	94	99	0.29	1	4
10	1	0.53	6	8	0.93	0	0	0.11	28	61	0.31	0	5
50	10	0.32	8	20	0.89	0	0	0.48	0	0	0.79	0	0
40	10	0.38	5	11	0.92	0	0	0.46	0	0	0.81	0	0
30	10	0.34	6	10	0.92	0	0	0.38	0	1	0.77	0	0
20	10	0.34	4	12	0.94	0	0	0.29	0	4	0.72	0	0
10	10	0.34	10	19	0.98	0	0	0.31	1	7	0.63	0	0
50	5	0.38	3	12	0.81	0	0	0.15	10	32	0.64	0	0
40	5	0.39	9	12	0.82	0	0	0.12	21	43	0.63	0	0
30	5	0.37	7	17	0.84	0	0	0.09	32	59	0.60	0	0
20	5	0.40	7	15	0.88	0	0	0.07	40	72	0.52	0	0
10	5	0.38	11	17	0.96	0	0	0.14	15	37	0.45	0	0
50	2	0.43	3	11	0.69	0	0	0.02	96	99	0.47	0	0
40	2	0.44	5	8	0.71	0	0	0.01	95	99	0.45	0	0
30	2	0.47	7	11	0.75	0	0	0.02	95	100	0.43	0	1
20	2	0.42	4	13	0.80	0	0	0.02	94	100	0.35	0	1
10	2	0.46	8	9	0.94	0	0	0.10	33	60	0.34	0	2
5	1	0.42	5	13	1.00	0	0	0.70	0	0	0.67	0	0
3	1	0.30	10	17	1.00	0	0	0.99	0	0	0.98	0	0
1	1	0.20	18	38	1.00	0	0	1.00	0	0	1.00	0	0